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Automatic computation of knots and weights of cubature formulae for circular symmetric planar regions

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Abstract: We are concerned with the construction of high degree formulae for circular symmetric planar regions, such as a circle and the entire plane. With the aid of invariant polynomials with respect to reflection groups, we decompose the problem into relative small quadrature problems. The cubature formulae can be constructed by an automatic procedure.

Keywords: Cubature formulae, invariant polynomial.

1. Introduction

Cubature formulae can be constructed by solving a system of moment equations. The number of equations and unknowns in these systems of nonlinear equations grows very rapidly with the degree of the cubature formulae and the dimension of the integral.

The usual way to reduce the number of equations and unknowns is to impose some structure on the formula. Invariant polynomials with respect to transformation groups turn out to be a very useful tool to attack the problem. In this paper, we first give an introduction to invariant theory. Then we use it to construct high degree cubature formulae for some two dimensional regions.

2. Transformation groups and invariant polynomials

2.1. Introduction

Let G be a group of linear transformations acting on a finite dimensional vector space V over a field K. A set $\Omega \subset V$ is said to be *invariant with respect to a group* G, if $g(\Omega) = \Omega$ for any $g \in G$. A function $\phi(x)$, defined on V is said to be *invariant with respect to the group* G if $\phi(g(x)) = \phi(x)$ for any $g \in G$ and $x \in V$. If $\phi(x)$ is a polynomial function, $\phi(x)$ is called an *invariant polynomial with respect to* G.

Polynomials $\psi_1(x), \ldots, \psi_r(x)$ are called *algebraically dependent* if there is a polynomial $\psi(x)$ in r variables with complex coefficients, not all zero, such that $\psi(\psi_1(x), \ldots, \psi_r(x)) \equiv 0$. Otherwise $\psi_1(x), \ldots, \psi_r(x)$ are called *algebraically independent*.

A linear transformation acting on the n-dimensional vector space V is said to be a *reflection* if it fixes an $n-1$ dimensional hyperplane. G is a *reflection group* if it is generated by reflections. The set of points $g(a)$, where $a \in V$ is fixed, and g runs through all elements of a group G, is called a *G-orbit* containing the point a.

Let $I_1(x), \ldots, I_l(x)$ be invariant polynomials of G. $I_1(x), \ldots, I_l(x)$ forms an *integrity basis* for the invariant polynomials of $G \Leftrightarrow$ any polynomial invariant under G is a polynomial in $I_1(x), \ldots, I_l(x)$. Each polynomial I_i is called a *basic invariant polynomial of* G.

Theorem 1. *Let G be a finite reflection group acting on the n-dimensional vector space V over a field K of characteristic* 0. *The invariant polynomials of G have an integrity basis consisting of n homogeneous elements which are algebraically independent over K.*

Proof. See Chevalley [1]. □

More about invariant polynomials can be found in Flatto [3].

2.2. *Invariant polynomials for dihedral groups*

Let G be the symmetry group of a regular polygon with the origin as center and invariant under reflection through the x-axis, on the vector space $\mathbb{R}^2$. G is a reflection group. The symmetry group of this regular N-gon contains N rotations and N reflections. It is known as the *dihedral group D_N of order 2N.*

Theorem 2. *The basic invariant polynomials of D_N can be chosen as $\sigma_2 = r^2$ and $\sigma_N = r^N \cos N\theta$ where $x = r\cos\theta$ and $y = r \sin\theta$.*

Proof. See Cools and Haegemans [2]. □

3. Invariant cubature formulae

3.1. *Introduction*

We are concerned with determining the knots (x_i, y_i) and weights w_i in a cubature formula

$$Q[f] = \sum_{i=1}^{M} w_i f(x_i, y_i) \tag{1}$$

which is an approximation of

$$I[f] = \int_R\int w(x, y) f(x, y)\, \mathrm{d}x\, \mathrm{d}y.$$

A cubature formula is said to be *invariant with respect to a transformation group G*, if the domain of integration R and the weight function $w(x, y)$ are invariant with respect to G, and if the set of knots is a union of G-orbits, where the knots of one and the same orbit have the same coefficient w_i.

The vector space of all polynomials in x and y of degree $\leqslant n$ is denoted by P_n. A cubature formula which is exact for all $P \in P_m$ but not for all $P \in P_{m+1}$, is said to have *degree m.*

Theorem 3. *Let the formula* (1) *be invariant with respect to G. In order for the formula* (1) *to be exact for all polynomials in* P_m *it is necessary and sufficient that* (1) *is exact for all those polynomials which are invariant with respect to G.*

Proof. See Sobolev [8]. □

From Theorem 2 and 3 follows that an invariant cubature formula with respect to D_N has degree m if and only if the formula is exact for

$$(r^2)^i \cdot (r^N \cdot \cos N\theta)^j \quad \forall i, j \in \mathbb{N} \text{ and } 2i + jN \leqslant m.$$

It is also necessary and sufficient that the formula is exact for the polynomials

$$r^{jN+2i} \cdot \cos(jN\theta) \quad \forall j, i \in \mathbb{N} \text{ and } jN + 2i \leqslant m.$$

A region is called *circular symmetric* if the region R and the weight function $w(x, y)$ remain unchanged under the linear transformation $x' = x \cdot \cos\theta + y \cdot \sin\theta$, $y' = -x \cdot \sin\theta + y \cdot \cos\theta$ where θ is arbitrary. For such regions

$$I\left[r^{j+2l}\cos(j\theta)\right] = 0 \quad \forall j \in \mathbb{N}_0, \quad l \in \mathbb{N}.$$

From now on, we only consider circular symmetric regions.

A *basic* D_N *cubature rule operator* Q_N (r, α) is defined as

$$Q_N(r, \alpha)f = \frac{1}{2N}\sum_{j=0}^{N-1}\left(f\left(r, \alpha + \frac{2\pi j}{N}\right) + f\left(r, -\alpha + \frac{2\pi j}{N}\right)\right)$$

with f a function of the polar coordinates r and θ. $Q_N(r, \alpha)f$ requires
- 1 function evaluation if $r = 0$,
- N function evaluations if $\cos(2N\alpha) = 1$, and
- $2N$ function evaluations otherwise.

(This concept is from Lyness and Jespersen [7]). We only consider cubature formulae with basic rule operators with $r = 0$ or $\cos(2N\alpha) = 1$.

3.2. Circular symmetric cubature formulae for circular symmetric regions

We search for cubature formulae of the form

$$Q[f] = \sum_{i=1}^{\text{nmax}} \sum_{t=1}^{a_i} w_{it} Q_{N_i}(r_{it}, \alpha_i) f + w_0 f(0, \cdot) \tag{2}$$

where

$$\begin{aligned} &N_1 = A \cdot 2, && \alpha_1 = 0, \\ &N_n = A \cdot 2^{n-1}, && \alpha_n = \pi/N_n, \quad n = 2, \ldots, \text{nmax} \quad \text{with } A \in \mathbb{N}_0 \setminus \{1\}. \end{aligned} \tag{3}$$

The cubature formulae constructed by Haegemans [5] are of this form. The main differences between [5] and this work are the theoretical approach, which lead to an automatic procedure, and the free parameter A, which can be choosen so that the cubature formula with the smallest number of knots is obtained.

Since the location of the knots is symmetric with respect to x- and y-axis, we only have to consider cubature formulae of odd degree $m = 2k - 1$. These formulae are invariant with respect to D_{N_1}. Because of the special structure, the number of polynomials for which the cubature formula must be exact can be further reduced.

Theorem 4. *A cubature formula* (2) *with the knots as specified in* (3) *has degree* $m = 2k - 1$ *if and only if the formula is exact for*

$$r^{2l}, \quad l = 0, \dots, k-1, \tag{4}$$

and

$$r^{N_n+2l}(1 - \cos N_n\theta), \quad n = 2, \dots, \text{nmax} \quad \text{and} \quad l = 0, \dots, k - 1 - \tfrac{1}{2}N_n \tag{5}$$

with

$$\begin{aligned} \text{nmax} &= 1 && \text{if } k-1 < A, \\ \text{nmax} &= 2 + \left[\log_2\left(\frac{k-1}{A}\right)\right] && \text{if } k-1 \geqslant A. \end{aligned}$$

Proof. See Cools and Haegemans [2] □

We assume that the moments

$$I\left[r^{2l}\right] = \mu_{2l}, \quad l = 0, \dots, k-1 \tag{6}$$

are known. A cubature formula of the form (3) has degree $2k - 1$ if it is exact for the polynomials (4) and (5). Each requirement gives us a non-linear equation. For each value of n in Theorem 4, we obtain a small system of nonlinear equations analogous to the system for determining a quadrature formula. The problem is now reduced from solving one large system of nonlinear equations to solving more, but smaller systems of nonlinear equations sequentially. The order in which the smaller systems must be solved is given in the following scheme:

(1) $j = \text{nmax} - 1$.

(2) While $j > 1$, solve the following system of nonlinear equations of type II.j (all the unknowns appear only in the left side):

$$2\sum_{t=1}^{a_{j+1}} w_{j+1,t} r_{j+1,t}^{N_{j+1}+2l} = \mu_{N_{j+1}+2l} - \sum_{i=j+2}^{\text{nmax}} \sum_{t=1}^{a_i} w_{it} r_{it}^{N_{j+1}+2l},$$
$$l = 0, \dots, k - 1 - \tfrac{1}{2}N_{j+1}. \tag{7}$$

(3) Solve the following system of nonlinear equations of type I (all the unknowns appear only in the lefts side):

$$\sum_{t=1}^{a_1} w_{1t} r_{1t}^{2l} = \mu_{2l} - \sum_{i=2}^{\text{nmax}} \sum_{t=1}^{a_i} w_{it} r_{it}^{2l}, \quad l = 0, \dots, k-1. \tag{8}$$

Solving a quadrature problem starting from the ordinary moments, is often called an ill conditioned problem. Note however that to determine a cubature formula of degree $m = 2k - 1$, the largest quadrature problem we must solve is the construction of a quadrature formula of degree $2[\frac{1}{2}k] - 1$.

The solution of the system of nonlinear equations can easily be found if the number of equations of type II.j is even. We only consider this case. The above scheme is translated into a FORTRAN 77 subroutine, CISYR [2], that computes automatically a cubature formula of a given degree m with given structure parameter A for a region for which the moments (6) are known.

3.3. Characteristics of the cubature formula

We summarize some characteristics of the cubature formulae. Details can be found in [2].

k even

- The number of equations of type II.j is even when A is even.
- The number of knots
$$K(k, A) = kA2^{\text{nmax}-1} - \tfrac{1}{3}A^2(4^{\text{nmax}-1} - 1) \text{ if nmax} \geqslant 2$$
and
$$K(k, A) = kA \quad \text{if nmax} = 1.$$
- For a given $k \leqslant 20$, the number of knots $K(k, A)$ is minimal if $A = 2$. If $k \geqslant 22$, the number of knots $K(k, 2)$ is not always minimal (e.g. $K(22, 6) < K(22, 2)$).

k odd

- The number of equations of type II.j is even when A is odd and $k \leqslant 2A - 1$.
- The number of knots
$$K(k, A) = -A^2 + (2k - 1)A + 1 \quad \text{if nmax} = 2$$
and
$$K(k, A) = A(k - 1) + 1 \text{ if nmax} = 1.$$
- For a given k, the number of knots $K(k, A)$ is minimal if
$$A = \tfrac{1}{2}(k + 1) + \tfrac{1}{2}(k \bmod 4 - 1).$$

3.4. In search of good formulae

Until now, we never asked ourselves if the systems of nonlinear equations (7) and (8) have a real solution, with knots inside the region and positive weights. In this paragraph we will partially answer this question.

For circular symmetric regions
$$\mu_{2l} = I[r^{2l}] = \int_0^R w(r) r^{2l}\, dr.$$
Thus, solving the nonlinear equations (7) for $j = \text{nmax} - 1$ is nothing else than solving a quadrature problem.

Theorem 5. *A cubature formula of the form* (2) *for a circular symmetric region with*
$$I[r^{2l}] = \int_0^R w(r) r^{2l}\, dr$$

with $w(r) \geqslant 0$ *for* $r \in [0, R]$, *that is obtained by solving equations* (7) *and* (8), *has*

$$w_{\mathrm{nmax},t} > 0 \quad \text{and} \quad 0 < r_{\mathrm{nmax},t} < R \quad \forall t \in \{1, \ldots, a_{\mathrm{nmax}}\}.$$

Proof. See Cools and Haegemans [2]. □

Theorem 5 is all we could prove about the knots and weights. Thus, if nmax > 1 we can not be sure that the solution of the equations (7) and (8) is real, with all knots inside the region and positive weights.

3.5. Applications

We are specially interested in the following circular symmetric regions:

$S_2^{a,b}$: the circle $\{(x, y): x^2 + y^2 \leqslant 1\}$ with weight function

$$w(x, y) = (x^2 + y^2)^{-a}(1 - x^2 - y^2)^{-b} \quad \text{with } a, b < 1.$$

$E_2^{r^a}$: the entire two-dimensional plane with weight function

$$w(x, y) = \mathrm{e}^{-(x^2+y^2)^{a/2}} \quad \text{with } a > 0.$$

Expressions for the moments (6) for these regions, are known:

$$S_2^{a,b}: \ \mu_{2l} = \pi \frac{\Gamma(l - a + 1)\Gamma(1 - b)}{\Gamma(l - a - b + 2)}.$$

$$E_2^{r^a}: \ \mu_{2l} = \frac{2\pi}{a} \Gamma\left(\frac{2l + 2}{a}\right).$$

The structure of the formulae constructed by Haegemans [5] is such that the number of knots $K(k, A)$ is minimal for a given $k \leqslant 16$. In [6] tables of these cubature formulae are given for the regions $S_2^{0,0}$, $E_2^{r^2}$ and E_2^r for $k \leqslant 16$. The formulae with minimal number of knots according to section 3.3, for the regions we are interested in and $k \leqslant 25$, have real knots that are inside the region and all weights positive, except when $k = 18$ and $K(18, 2) = 236$. When $k = 18$ there exist formulae with $A = 6$ and $K(18, 6) = 252$ real knots.

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